

Quantum criticality of the sub-Ohmic spin-boson model within displaced Fock states

Shu He¹, Liwei Duan¹, and Qing-Hu Chen^{1,2,*}

¹ *Department of Physics, Zhejiang University, Hangzhou 310027, P. R. China*

² *Center for Statistical and Theoretical Condensed Matter Physics, Zhejiang Normal University, Jinhua 321004, P. R. China*

(Dated: October 7, 2014)

The spin-boson model is analytically studied using displaced Fock states (DFS) without discretization of the continuum bath. In the orthogonal displaced Fock basis, the ground-state wavefunction can be systematically improved in a controllable way. Interestingly, the zeroth-order DFS reproduces exactly the well known Silbey-Harris results. In the framework of the second-order DFS, the magnetization and the entanglement entropy are exactly calculated. It is found that the magnetic critical exponent β is converged to 0.5 in the whole sub-Ohmic bath regime $0 < s < 1$, compared with that by the exactly solvable generalized Silbey-Harris ansatz. It is strongly suggested that the system with sub-Ohmic bath is always above its upper critical dimension, in sharp contrast with the previous findings. This is the first evidence of the violation of the quantum-classical Mapping for $1/2 < s < 1$.

PACS numbers: 03.65.Yz, 03.65.Ud, 71.27.+a, 71.38..k

The spin-boson model [1, 2] describes a qubit (two-level system) coupled with a dissipative environment represented by a continuous bath of bosonic modes. There are currently considerable interests in this quantum many-body system due to the rich physics of quantum criticality and decoherence [2–4], applied to the emerging field of quantum computations [5], quantum devices [6], and quantum biology [7, 8]. It is widely used to study the microscopic behavior of the open quantum systems [1]. The coupling between the qubit and the environment is characterized by a spectral function $J(\omega)$ which is proportional to ω^s . The spectral exponent s varies the coupling into three different cases: sub-Ohmic ($s < 1$), Ohmic ($s = 1$), and super-Ohmic ($s > 1$).

As a paradigmatic model to study the influence of environment on the quantum system, the spin-boson model has been extensively and persistently studied by many analytical and numerical approaches. On the analytical side, a pioneer work is undoubtedly the variational study based on the polaronic unitary transformation by Silbey-Harris (SH) ansatz [9]. Based on the GHZ ansatz, Zheng *et al.* developed an analytical approach [10] to study both static and dynamical behavior of the dissipative two-level system. Chin *et al.* generalized the Silbey-Harris (GSH) variational polaronic ansatz to a asymmetrically one in the sub-Ohmic spin-boson model [11]. All these studies are based on single coherent state in both levels. Recently, this single coherent states ansatz was improved by simply adding other coherent states on the equal footing [12] and by superpositions of two degenerate single coherent states [13]. By the way, the similar idea was also proposed by one of the present author and a collaborator in 2005 for single-mode case [14] independently.

On the numerical side, almost all advanced numerical approaches in the quantum many-particle physics have been applied and extended to this model. The numerical renormalization group (NRG) was applied at the earlier stage [15] for the sub-Ohmic baths, but the direct appli-

cations yields incorrect critical exponents of the quantum phase transitions (QPT) for $0 < s < 1/2$ and therefore invalidate the famous quantum-to-classical correspondence due to the Hilbert-space truncation error and the mass flow error [16–18]. Later on, quantum Monte Carlo simulations based on a imaginary path integral [19], sparse polynomial space approach [20], exact diagonalization in terms of shift bosons [21] have sequentially developed and all found the mean-field critical exponent for $0 < s < 1/2$. The density matrix renormalization group (DMRG) was also applied, but not successful in the analysis of the critical phenomena [22]. More recently, using the DMRG algorithm combined with the optimized phonon basis, a variational matrix product state (MPS) approach formulated on a Wilson chain [23] was developed and the Hilbert-space truncation can be alleviated systematically. Very recently, an alternative to the conventional MPS representation was also proposed [24]. For $1/2 < s < 1$, the magnetic critical exponent β obtained in two MPS approaches [23, 24] and the NRG [15, 17] is much less than 0.5, indicating that the system is below its upper critical dimension.

Among the numerical approaches to the celebrated continuum spin-boson model, the discretization of the energy spectrum of the bath should be performed at the very beginning, except for some approaches formulated on path integral [19] where the bath is analytically integrated out. Whether the artificial discretization will change the nature of the model system is still unclear. To ensure the convergence, the number of the bosonic modes then is set large enough so that the Hilbert-space truncation can be controlled systematically, and therefore the bath are described in a very complicated way, like in the various MPS approaches [23, 24] and NRG [15, 17]. To the best of our knowledge, the phonon state in the bath of the spin-boson model has not been analytically well described, except for approaches with more than one nonorthogonal coherent states [12, 13].

In this work, we propose an analytic ground state (GS) for the spin-boson model without discretization of the spectra. The phonon state is expanded in the novel orthogonal basis, and therefore described in a controllable way. The GS wavefunction can be obtained self-consistently, and all GS properties can then be numerically exactly calculated. The convergency of the criticality is discussed without ambiguity.

The Hamiltonian of the spin-boson model is given by

$$H = -\frac{\Delta}{2}\sigma_x + \sum_k \omega_k a_k^\dagger a_k + \frac{1}{2}\sigma_z \sum_k g_k (a_k^\dagger + a_k), \quad (1)$$

where σ_x and σ_z are Pauli matrices, Δ is the tunneling amplitude between two levels, ω_k and a_k^\dagger are the frequency and creation operator of the k -th harmonic oscillator, and g_k is the interaction strength between the k -th bosonic mode and the local spin. The spin-boson coupling is characterized by the spectral function,

$$J(\omega) = \pi \sum_k g_k^2 \delta(\omega_k - \omega) = 2\pi\lambda\omega_c^{1-s}\omega^s, 0 < \omega < \omega_c, \quad (2)$$

with ω_c a cutoff frequency. The dimensionless parameter λ denotes the coupling strength. The rich physics of the quantum dissipation is second-order QPT from delocalization to localization for $0 < s < 1$, as a consequence of the competition between the amplitude of tunneling of the spin and the effect of the dissipative bath.

To outline the approach more intuitively, we first consider the case without symmetry breaking, such as the delocalized phase. By using $|\uparrow\rangle$ and $|\downarrow\rangle$ to represent the eigenstate of σ_z , the GS wavefunction can be in principle expressed in the following set of complete orthogonal basis $\prod_{i=0}^n a_{k_i}^\dagger |0\rangle$

$$|\Psi'\rangle = \left(1 + \sum_k \alpha_k a_k^\dagger + \sum_{k_1, k_2} u_{k_1, k_2} a_{k_1}^\dagger a_{k_2}^\dagger + \dots\right) |0\rangle |\uparrow\rangle + \left(1 - \sum_k \alpha_k a_k^\dagger + \sum_{k_1, k_2} u_{k_1, k_2} a_{k_1}^\dagger a_{k_2}^\dagger + \dots\right) |0\rangle |\downarrow\rangle, \quad (3)$$

where $|0\rangle$ is vacuum of bath modes, $\alpha_k, u_{k_1 k_2}, \dots$ are the coefficients and even parity is considered. However, it is practically impossible to perform direct diagonalization in this way to get reasonable results, because very high order expansions is needed. Alternatively, the wavefunction (3) can be also expressed in terms of the other set of complete orthogonal basis, $D(\alpha_k) \prod a_{k_i}^\dagger |0\rangle$ with $D(\alpha_k) = \exp\left[\sum_k \alpha_k (a_k^\dagger - a_k)\right]$ a unitary operators

with displacement α_k given in Eq. (3), as

$$|\Psi\rangle = D(\alpha_k) \left(1 + \sum_{k_1, k_2} b_{k_1 k_2} a_{k_1}^\dagger a_{k_2}^\dagger + \dots\right) |0\rangle |\uparrow\rangle + D(-\alpha_k) \left(1 + \sum_{k_1, k_2} b_{k_1 k_2} a_{k_1}^\dagger a_{k_2}^\dagger + \dots\right) |0\rangle |\downarrow\rangle, \quad (4)$$

where the linear term $a_k^\dagger |0\rangle$ should be absent because the expansion of the whole phonon state of each level in the Fock space can completely reproduce the first two terms in Eq. (3). Note above that the phonon state in each level is generated by operating on the Fock state with a unitary displacement operators, thus we call it as displaced Fock states (DFS). Only the first term $D(\pm\alpha_k) |0\rangle$ can reach the whole Hilbert-space, so no truncation is made in this sense. If the expansion is taken to infinity, a exact solution would be obtained. In other words, the true wavefunction should take the form of Eq. 4). However, it is impossible to really perform an infinite expansion. Even for a few terms expansion, it is very time consuming. Fortunately, it will be shown later that only two terms in the expansion would give the converging results in some important issues.

First, as a zeroth-order DFS, we only consider the first term in Eq. (4). Projecting the Schrödinger equation onto the orthogonal states $\langle 0| D^\dagger(\alpha_k)$ and $\langle 0| a_k D^\dagger(\alpha_k)$ gives

$$\sum_k \omega_k \alpha_k^2 + \sum_k g_k \alpha_k - \frac{\Delta}{2} \exp\left[-2 \sum_k \alpha_k^2\right] = E, \quad (5)$$

$$\omega_k \alpha_k + \frac{1}{2} g_k + \Delta \exp\left[-2 \sum_k \alpha_k^2\right] \alpha_k = 0, \quad (6)$$

where we have used the properties of the unitary displacement operators

$$D^\dagger(\alpha_k) a_k^\dagger D(\alpha_k) = a_k^\dagger + \alpha(k); \quad D^\dagger(\alpha_k) a_k D(\alpha_k) = a_k + \alpha(k).$$

Eq. (6) immediately yields

$$\alpha_k = \frac{-\frac{1}{2}g_k}{\omega_k + \Delta \exp(-2 \sum_k \alpha_k^2)}, \quad (7)$$

Interestingly, this is just the SH result, although here it is not obtained through a variational scheme. So we arrive at the right track of the previous well-known analytical results only by the zeroth-order approximation. The advantage of the this technique is that we can easily go further to get more accurate results in a controllable way, by both modifying the displacement of the unitary operators and adding the correlations among different bosonic modes step by step.

In the second-order DFS, we only keep two terms in Eq. (4). Similarly, projecting the Schrödinger equation onto

$\langle 0|D^\dagger(\alpha_k)$, $\langle 0|a_{k_1}D^\dagger(\alpha_k)$, and $\langle 0|a_{k_1}a_{k_2}D^\dagger(\alpha_k)$ yields the following three equations for unknown E, α_k , and b_{k_1, k_2} ,

$$E = \sum_k (\omega_k \alpha_k^2 + g_k \alpha_k) - \frac{1}{2} \Delta \eta \left(1 + 4 \sum_k B_k \alpha_k \right), \quad (8)$$

$$\alpha_k = -\frac{\frac{g_k}{2} + 2 \sum_{k'} b_{k, k'} [(\omega_{k'} - \Delta \eta) \alpha_{k'} + \frac{g_{k'}}{2}]}{\omega_k + \Delta \eta (1 + 4 \sum_k B_k \alpha_k)}, \quad (9)$$

$$b_{k_1, k_2} = -\frac{B_{k_1} \alpha_{k_2} + B_{k_2} \alpha_{k_1} - \alpha_{k_1} \alpha_{k_2} (1 + 4 \sum_k B_k \alpha_k)}{2 \sum_k B_k \alpha_k + (\omega_{k_1} + \omega_{k_2}) / (\Delta \eta)}, \quad (10)$$

where

$$B_k = \sum_{k'} b_{k, k'} \alpha_{k'},$$

$$\eta = \exp \left[-2 \sum_k \alpha_k^2 \right].$$

Both $\alpha(k)$ and b_{k_1, k_2} can be obtained by solving the two coupled equations (9) and (10) self-consistently, which in turn give the GS energy and wavefunction. In our opinion, this is actually a parameter-free analytical approach.

Due to the QPT from the delocalized phase to the localized one in the sub-Ohmic spin-boson model, we should relax wavefunctions (4) to the asymmetrical one

$$|\Psi\rangle = D(\alpha_k) \left(1 + \sum_{k_1, k_2} b_1(k_1, k_2) a_{k_1}^\dagger a_{k_2}^\dagger + \dots \right) |0\rangle |\uparrow$$

$$+ D(\beta_k) \left(r + \sum_{k_1, k_2} b_2(k_1, k_2) a_{k_1}^\dagger a_{k_2}^\dagger + \dots \right) |0\rangle |\downarrow\rangle, \quad (11)$$

where r is the asymmetrical parameter. If $r = 1$ and $\beta_k = -\alpha_k$, the previous symmetrical results are recovered.

The zero-order DFS will give the same results as that in generalized SH polaronic ansatz [11], then it is also called the GSH ansatz in the remaining of the paper. In the second-order DFS, we have double equations for the counterparts in the symmetrical case. The number of unknown parameters are also doubled, due to the asymmetrical coefficients. We leave detailed derivations to Appendix A.

Proceeding as the scheme outlined above, we can straightforwardly perform the further expansion in the orthogonal displaced Fock basis $D(\alpha_k) \prod a_{k_i}^\dagger |0\rangle$ in the controllable way, and obtain the solution within any desired accuracy in principle. The challenges remain on the pathway to high dimensional integral in the further extensions, due to both the analytical derivations and exponentially increasing computational difficulties. On the other hand, the criterion of the precise description of the criticality can be that the further correction does

not change the nature in the last approximation. Fortunately, it will be shown later that the second-order correction really does not changes the critical exponents in the GSH ansatz at all, so the further corrections to the second-order DFS is not necessary, at least in the sense of the criticality.

The magnetization $\langle \sigma_z \rangle$ can be used as an order parameter in the QPT of this model. It shows a power law behavior near the critical point,

$$\langle \sigma_z \rangle \propto (\lambda - \lambda_c)^\beta. \quad (12)$$

The entanglement entropy between the qubit and the bath is defined as [25]

$$S = -Tr \rho_A \log_2 \rho_A = -Tr \rho_B \log_2 \rho_B,$$

$$\rho_{A(B)} = Tr_{B(A)} \langle \Psi | \Psi \rangle,$$

where A is the qubit and B is the bath, Ψ is the GS wavefunction of the whole system. In the spin-boson model, it is [4]

$$S = -p_+ \log_2 p_+ - p_- \log_2 p_-,$$

where

$$p_\pm = \left(1 \pm \sqrt{\langle \sigma_x \rangle^2 + \langle \sigma_z \rangle^2} \right) / 2.$$

We stress here that in the present approach we do not need to discretize the bosonic energy band like in many previous studies at the very beginning. All k -summation in the coupled equations can be transformed into continuous integral like $\int_0^{\omega_c} d\omega J(\omega) I(\omega)$. In this work, all integrals are numerically calculated within a Gaussian-logarithmical (GL) integration with very high accuracy. The detailed demonstration is given in Appendix B. Without loss of generality, we set $\Delta = 0.1, \omega_c = 1$ in the calculation throughout this paper, if not specified.

First, we calculate the magnetization and evaluate the critical points within both the GSH and the second-order DFS. The results for $s = 0.2, 0.4, 0.6$, and 0.8 are presented in Fig. 1 (a) by the solid lines (second-order DFS) and dashed lines (GSH). Both shows that there exist a critical point which separate the delocalized phase ($\langle \sigma_z \rangle = 0$) to the localized one ($\langle \sigma_z \rangle \neq 0$). The critical coupling strengths λ_c by the second-order DFS are larger than those by GSH, the correction becomes remarkable for $s > 0.5$. It follows that the GSH critical point will be modified by the second-order DFS. To determine the critical point within the second-order DFS more precisely, we also calculate the entanglement entropy, which exhibits a cusp characteristics around the critical point. The results are given in Fig. 1(b). Both the magnetization and the entanglers entropy result in the consistent value for the QPT critical point.

It should be pointed out that that the critical coupling strength obtained in the second-order DFS is not the true one in this model either, because it will be definitely revised by the third-order DFS, although the revision

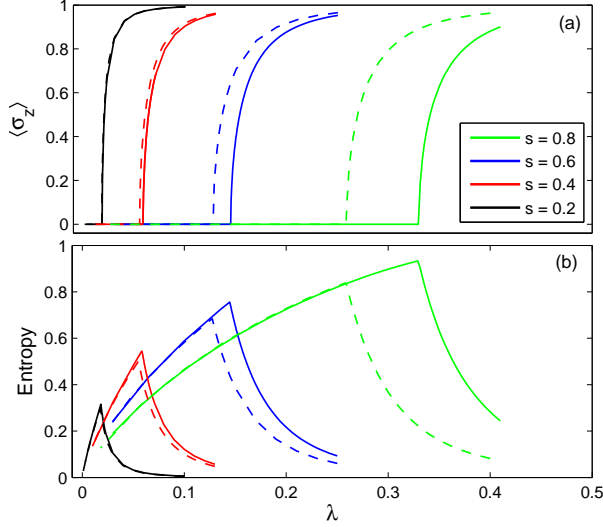


FIG. 1: (Color online) The magnetization and the entanglement entropy as a function the coupling strength within the GSH (dashed lines) and the second order DFS (solid lines) for $s = 0.2, 0.4, 0.6$, and 0.8 .

is probably small. It is expected that the converging critical point would be only obtained in the high-order DFS, which is however a challenging task at the moment, and also beyond the scope of the present study. The more crucial issue in a QPT is the criticality. So the natural question is "the criticality described by GSH could be changed in second-order DFS?"

In Fig. 2, we present the magnetization within both GSH and the second-order DFS as a function of $\lambda/(\lambda - \lambda_c)$ in a log-log plot for $s = 0.2, 0.4, 0.6$, and 0.8 . It is demonstrated that, using both approaches, the magnetic critical exponent β is always 0.5 with an error bar $(-0.01, 0.01)$, even for $s = 0.6$ and 0.8 . Note that the second-order DFS should be the dominate correction to the GSH, as indicted in the critical points. But for the critical exponent, we do not find any visible deviation from the GSH ones. We can not imagine that the further corrections would change this observation but the second-order correction does not. It is therefore strongly suggested that even in $s > 1/2$, the magnetic exponent β in the sub-Ohmic spin-boson model is always 0.5 , quite different from those obtained in the MPS [23, 24] and NRG [15, 17].

In summary, a new analytic approach referred to DFS is proposed in the spin-boson model with the continuum spectral function. The zero-order approximation is just the well known SH approach, the further corrections can be performed step by step. For the sub-Ohmic baths, the second-order DFS can modify the GSH critical coupling strength of the QPT, especially for $s > 1/2$. But the critical exponent is not changed at all, and is always 0.5 for the whole bath regime $0 < s < 1$, a mean-field value for the system above the upper critical dimension. This is a direct strict evidence of failure of quantum-classical

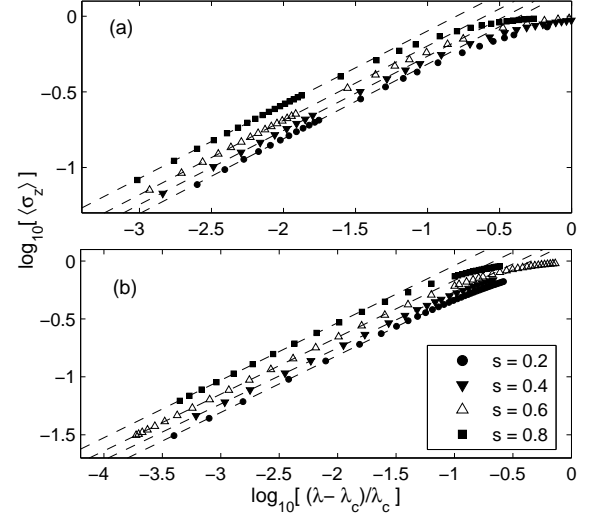


FIG. 2: The log-log plot of the magnetization $\langle \sigma_z \rangle$ as a function the coupling strength within the GSH and the second order DFS for $s = 0.2, 0.4, 0.6$, and 0.8 . $\omega_c = 1$, $\Delta = 0.1$

mapping in the sub-ohmic spin-boson model, at least for $s > 1/2$.

Outlook. It is expected that the sufficient number of integral grids for the converged results increases exponentially with the further corrections in the DFS. The Monte Carlo integral might be used in the high dimensional integral. But the analytical derivation in the high order DFS is also challenging task. New methods, probably like some diagrammatic techniques, in the framework of the DFS is highly called for. The progress along this avenue may hopefully lead to a true exact solution to this celebrated model, which is perhaps our future ambitions.

Because each summation over k in the final expressions is related to $\sum_k g_k^2$, we propose a discretized spin-boson Hamiltonian ($\omega_c = 1$) as follows

$$H = -\frac{\Delta}{2}\sigma_x + \sum_k \omega_k a_k^\dagger a_k + \frac{1}{2}\sigma_z \sum_k \sqrt{\frac{W(\omega_k)J(\omega_k)}{\pi}}(a_k^\dagger + a_k), \quad (13)$$

where $\omega_k = \omega_{m,n}$ is the Gaussian integration point in Eq. (B5), $W(\omega_k)$ is the Gaussian weight. Applying the present DFS approach to this Hamiltonian, all results obtained in this paper are recovered completely by direct summation over k . It is shown in Appendix B that a limited number of discretizations can give results with very high accuracy. In this sense, Hamiltonian (13) is equivalent to the model for one qubit coupled with a finite number bosonic modes, which facilitates the further study. We believe that Eq. (13) with discretized bosonic modes could be a new starting Hamiltonian for any advanced approaches. The dynamics based on polaron trial state by the name of the Davydov D1 ansatz within the Dirac-Frenkel time dependent variational procedure [26] can be revisited using the discretized one directly.

This work is supported by National Natural Science

Foundation of China under Grant No. 11474256, and National Basic Research Program of China under Grant No. 2011CBA00103.

* Corresponding author. Email:qhchen@zju.edu.cn

where

Appendix A: DFS for the sub-Ohmic baths

In the zeroth order approximation, we only select the first term Eq. (11). Similar to the derivation in the symmetric case, projecting the Schrödinger equation in the upper level onto the orthogonal basis $\langle 0| D^\dagger(\alpha_k)$ and $\langle 0| a_k D^\dagger(\alpha_k)$ and low level onto $\langle 0| D^\dagger(\beta_k)$ and $\langle 0| a_k D^\dagger(\beta_k)$ result in

$$\sum_k (\omega_k \alpha_k^2 + g_k \alpha_k) - \frac{\Delta}{2} r \Gamma = E, \quad (\text{A1})$$

$$\omega_k \alpha_k + \frac{1}{2} g_k + \frac{\Delta}{2} r \Gamma D_k = 0, \quad (\text{A2})$$

and

$$\sum_k (\omega_k \beta_k^2 - g_k \beta_k) - \frac{\Delta}{2r} \Gamma = E, \quad (\text{A3})$$

$$\omega_k \beta_k - \frac{1}{2} g_k - \frac{\Delta}{2r} \Gamma D_k = 0, \quad (\text{A4})$$

which are the same as those obtained variationally within the GSH ansatz [11].

For the second-order DFS, the first two terms in Eq. (11) is kept. Proceeding as procedures outlines above, Projecting the Schrödinger equation in the upper level onto the orthogonal states $\langle 0| D^\dagger(\alpha_k)$, $\langle 0| a_k D^\dagger(\alpha_k)$, and $\langle 0| a_{k_1} a_{k_2} D^\dagger(\alpha_k)$ and low level onto $\langle 0| D^\dagger(\beta_k)$, $\langle 0| a_k D^\dagger(\beta_k)$, and $\langle 0| a_{k_1} a_{k_2} D^\dagger(\beta_k)$ yield the following six equations

$$\sum_k [\omega_k \alpha_k^2 + g_k \alpha_k] - \frac{\Delta}{2} \Gamma \left[r + \sum_k B_k D_k \right] = E, \quad (\text{A5})$$

$$r \sum_k [\omega_k \beta_k^2 - g_k \beta_k] - \frac{\Delta}{2} \Gamma \left[1 + \sum_k A_k D_k \right] = rE, \quad (\text{A6})$$

$$\left[\omega_k \alpha_k + \frac{g_k}{2} \right] + \sum_{k'} 2b_1(k, k') \left[\omega_{k'} \alpha_{k'} + \frac{g_{k'}}{2} \right] - \Delta \Gamma B_k + \frac{\Delta}{2} \Gamma D_k \left[r + \sum_k B_k D_k \right] = 0, \quad (\text{A7})$$

$$r \left[\omega_k \beta_k - \frac{g_k}{2} \right] + \sum_{k'} 2b_2(k, k') \left[\omega_{k'} \beta_{k'} - \frac{g_{k'}}{2} \right] + \Delta \Gamma A_k - \frac{\Delta}{2} \Gamma D_k \left[1 + \sum_k A_k D_k \right] = 0, \quad (\text{A8})$$

$$b_1(k_1, k_2) (\omega_{k_1} + \omega_{k_2}) + \frac{\Delta}{2} \Gamma \left[r + \sum_k B_k D_k \right] b_1(k_1, k_2) - \frac{\Delta}{2} b_2(k_1, k_2) \Gamma + \frac{\Delta}{2} \Gamma [B_{k_1} D_{k_2} + B_{k_2} D_{k_1}] - \frac{\Delta}{4} \Gamma D_{k_1} D_{k_2} \left[r + \sum_k B_k D_k \right] = 0, \quad (\text{A9})$$

$$b_2(k_1, k_2) (\omega_{k_1} + \omega_{k_2}) + \frac{\Delta}{2r} \Gamma \left[1 + \sum_k A_k D_k \right] b_2(k_1, k_2) - \frac{\Delta}{2} b_1(k_1, k_2) \Gamma + \frac{\Delta}{2} \Gamma [A_{k_1} D_{k_2} + A_{k_2} D_{k_1}] - \frac{\Delta}{4} \Gamma D_{k_1} D_{k_2} \left[1 + \sum_k A_k D_k \right] = 0, \quad (\text{A10})$$

where

$$A_k = \sum_{k'} b_1(k', k) D_{k'},$$

$$B_k = \sum_{k'} b_2(k', k) D_{k'}.$$

The self-consistent solutions for the four coupled equa-

tions Eqs. (A7), (A8), (A9) and (A10) will give all results in the second-order DFS. If set $r = 1, \alpha_k = -\beta_k$ and $b_1(k_1, k_2) = b_2(k_1, k_2)$, Eqs. (9) and (10) in the symmetric case are recovered completely.

Appendix B: Gaussian-logarithmical integration for the continuous integral

The symmetrical case is also used to illustrate a effective numerical approach to the calculation of the summation clearly. In the zeroth-order approximation, also the well known SH ansatz, we can set

$$\alpha_k = \alpha'_k g_k,$$

Eq. (7) becomes

$$\alpha'_k = -\frac{1/2}{\omega_k + \Delta \exp(-2 \sum_k \alpha_k'^2 g_k^2)},$$

so α'_k is only related to g_k implicitly.

According to the spectral density, we have

$$\alpha'(\omega) = -\frac{1/2}{\omega + \Delta \exp\left[-\frac{2}{\pi} \int_0^{\omega_c} d\omega' \alpha'^2(\omega') J(\omega')\right]}, \quad (\text{B1})$$

which can be solved numerically by iterations.

In the second-order approximation, we can set

$$\begin{aligned} \alpha_k &= \alpha'_k g_k, \\ b_{k_1, k_2} &= b'_{k_1, k_2} g_{k_1} g_{k_2}. \end{aligned}$$

Inserting to Eqs. (9) and (10) gives

$$\alpha'_k = \frac{-\frac{1}{2} + 2 \sum_{k'} g_{k'}^2 b'_{k, k'} [(\omega_{k'} - \Delta\eta) \alpha'_{k'} + 1/2]}{\omega_k + \Delta\eta (1 + 4\zeta)},$$

$$b'_{k_1, k_2} = \frac{\alpha'_{k_1} \alpha'_{k_2} (1 + 4\zeta) - \sum_{k'} g_{k'}^2 \alpha'_{k'} (b'_{k_1, k'} \alpha'_{k_2} + b'_{k_2, k'} \alpha'_{k_1})}{2\zeta + (\omega_{k_1} + \omega_{k_2}) / (\Delta\eta)}$$

where

$$\zeta = \sum_k g_k^2 \sum_{k'} g_{k'}^2 b'_{k, k'} \alpha'_{k'} \alpha'_k.$$

Given g_k , both α'_k and b'_{k_1, k_2} can be obtained self-consistently. Note that each k -summation takes the form of $\sum_k g_k^2 I(k)$ where $I(k)$ does not depend on g_k^2 explicitly, and so both α'_k and b'_{k_1, k_2} are functionals of g_k . Without loss of generality, k is corresponding to ω one by one, the k -summation can be transformed to the ω integral as

$$\sum_k g_k^2 I(k) \rightarrow \int_0^{\omega_c} d\omega \frac{J(\omega)}{\pi} I(\omega),$$

so we have

$$\alpha'(\omega) = \frac{-\frac{1}{2} + \xi(\omega) - 2\Delta\eta\chi(\omega)}{\omega + \Delta\eta (1 + 4\zeta)}, \quad (\text{B2})$$

$$b'(\omega_1, \omega_2) = \frac{\alpha'(\omega_1) \alpha'(\omega_2) (1 + 4\zeta) - \kappa(\omega_1, \omega_2)}{2\zeta + (\omega_1 + \omega_2) / (\Delta\eta)}, \quad (\text{B3})$$

where

$$\xi(\omega) = \int_0^{\omega_c} d\omega' \frac{J(\omega')}{\pi} [2\omega' \alpha'(\omega') + 1] b'(\omega, \omega'),$$

$$\chi(\omega) = \int_0^{\omega_c} d\omega' \frac{J(\omega')}{\pi} \alpha'(\omega') b'(\omega, \omega'),$$

$$\kappa(\omega_1, \omega_2) = \chi(\omega_1) \alpha'(\omega_2) + \chi(\omega_2) \alpha'(\omega_1),$$

are some functions for ω , and

$$\zeta = \int_0^{\omega_c} d\omega \frac{J(\omega)}{\pi} \int_0^{\omega_c} d\omega' \frac{J(\omega')}{\pi} \alpha'(\omega) \alpha'(\omega') b'(\omega, \omega'),$$

$$\eta = \exp\left[-2 \int_0^{\omega_c} d\omega' \frac{J(\omega')}{\pi} \alpha'^2(\omega')\right],$$

are constants. If both $\alpha'(\omega)$ and $b'(\omega_1, \omega_2)$ are obtained, all observables can in turn be calculated. For example, using Eq. (8), the energy in the second-order DFS can be calculate as

$$E = \int_0^{\omega_c} d\omega \frac{J(\omega)}{\pi} \alpha'(\omega) [\omega \alpha'(\omega) + 1] - \frac{1}{2} \Delta\eta (1 + 4\zeta). \quad (\text{B4})$$

The self-consistent solutions in the coupled equations Eqs. (B2) and (B3)) are in no way obtained analytically, numerical calculation should be performed. Note that the low frequency modes play the dominant role in the QPT of the sub-ohmic spin-boson model. At the critical point, there is an infrared divergence of the integrand like $\int_0^{\omega_c} \omega^{s-2} d\omega$ in the limit of $\omega \rightarrow 0$ for sub-ohmic bath, which is called as the infrared catastrophe. Thanks to the Gaussian quadrature rules, where the zero frequency is not touched. We can discretize the whole frequency interval with Gaussian grids, the integral can be numerically exactly achieved with a large number of Gaussian grids. It is very time consuming to calculate the integral in this way, especially for high dimensional integral involved in the high-order DFS. According to the structure of the integrand, it is not economical to deal with the high and low frequency regime on the equal footing. To increase the efficiency, we combine the logarithmic discretization and Gaussian quadrature rule. First, we divide the ω interval $[0, 1]$ into $M + 1$ sub-intervals as $[\Lambda^{-(m+1)}, \Lambda^{-m}]$ ($m = 0, 1, 2, M - 1$) and $[0, \Lambda^{-M}]$, then we apply the Gaussian quadrature rule to each logarithmical sub-interval. So the continuous integral is calculated by the following summation

$$\int_0^1 J(\omega) I(\omega) d\omega = \sum_{m=0}^M \sum_{n=1}^N W_{m,n} J(\omega_{m,n}) I(\omega_{m,n}), \quad (\text{B5})$$

where N is the number of gaussian points inserted in each sub-interval, $W_{m,n}$ is corresponding Gaussian weight.

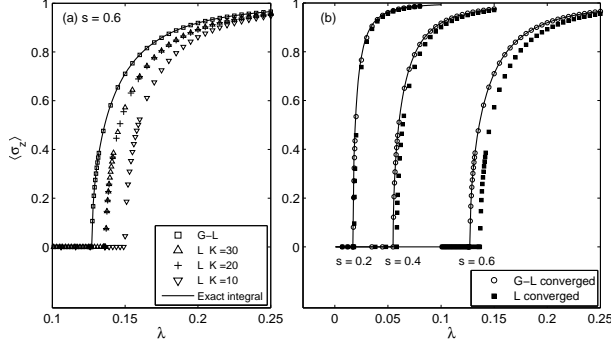


FIG. 3: Magnetization $\langle \sigma_z \rangle$ as a function of the coupling strength λ in the GSH ansatz. (a) For $s = 0.6$, converged results within GL integration (open squares), numerical exact ones (solid lines), and those within logarithmic discretization with different truncation numbers $K = 10, 20$, and 30 . (b) The converged magnetization within GL integration (open circles) and logarithmic discretization (filled squares) for $s = 0.2, 0.4$, and 0.6 . Numerical exact ones are denoted by the solid lines.

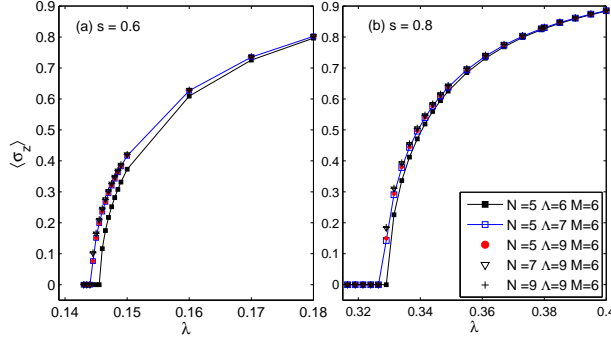


FIG. 4: (Color online) Magnetization $\langle \sigma_z \rangle$ as a function of the coupling strength λ in the second-order DFS within GL integration using different M, N , and Λ for (a) $s = 0.6$ and (b) $s = 0.8$.

To demonstrate the efficiency of the Gaussian-logarithmical (GL) integration, we first apply it to the GSH ansatz, which is also the zero-order approximation in the DFS. The one-dimensional integral can be numerically exactly done by Gaussian integration over the whole interval with a huge number of discretizations, and corresponding results can be regarded as a benchmark. After careful examinations, using the GL technique, the converging results for the magnetization can be archived if

set $M = 6, N = 9$, and $\Lambda = 9$. The corresponding results for $s = 0.6$ are presented in Fig. 3 (a) with open squares, which agrees excellently with the numerically exact one by a huge number of discretization in the Gaussian integration (solid lines).

We can also perform the logarithmic discretization of the bosonic energy band, as was widely used in the previous studies, such as NRG [15] and multi-coherent states [12]. In the GSH ansatz, this can be easily done by set

$$g_k^2 = \int_{\Lambda^{-(k+1)}}^{\Lambda^{-k}} \frac{J(\omega)}{\pi} d\omega, \quad \omega_k = \frac{1}{g_k} \int_{\Lambda^{-(k+1)}}^{\Lambda^{-k}} \frac{J(\omega)}{\pi} \omega d\omega, \quad (\text{B6})$$

in Eqs. (A1-A4) of Appendix A. The spectral density is truncated to a number K of modes. The summation is performed over the integer k directly and the self-consistent solution with discretized form can be also obtained. The logarithmic grid is chosen as $\Lambda = 2$, the same as that in Refs. [12, 15]. The magnetization as a function of λ for $s = 0.6$ with such a logarithmic discretization are collected in Fig. 3 (a) with different truncation number K of bosonic modes. The converging results can be also obtained for $K \geq 20$, which is however obviously different from the numerically exact one. Note that this kind of logarithmic discretization of the bosonic energy band at the very beginning is not equivalent to the logarithmic discretization of the continuous integral derived in the end of the DFS approach.

The converged magnetization within both the GL and logarithmic discretization for different values of s are carefully examined, and the results are exhibited in Fig. 3 (b). The deviation between these two convergent ones increases with s , and becomes remarkable for $s \geq 0.3$.

Then we turn to the second-order DFS study, a central issue in this work. Two-dimensional integral will be involved in this case, so direct Gaussian integral with huge number of discretization is practically difficult. Fortunately, it has been convincingly shown above that in the framework of GSH ansatz, the Gaussian-logarithmic discretization with dozens of grids to the continuous integral can effectively give results with very high accuracy. Therefore we extend this numerical technique to the present case. Interestingly, an excellent convergence behavior for $s = 0.6$ (a) and $s = 0.8$ (b) is demonstrated in Fig. 4 with different value of M, N , and Λ . The converged results obtained in this way compose the main achievement in this work.

-
- [1] A. J. Leggett et al., Rev. Mod. Phys. **59**, 1(1987).
 - [2] U. Weiss, Quantum Dissipative Systems (World Scientific, Singapore, 1993).
 - [3] K. L. Hur, P. D. Beaupré, and W. Hofstetter, Phys. Rev. Lett. **99**, 126801(2007).
 - [4] A. Kopp and K. Le Hur, Phys. Rev. Lett. **98**, 220401

- (2007)
- [5] M. Thorwart and P. Hanggi, Phys. Rev. A **65**, 012309 (2001); T. A. Costi and R. H. McKenzie, Phys. Rev. A **68**, 034301 (2003).
- [6] Y. Makhlin, G. Schon, and A. Shnirman, Phys. Mod. Phys. **73**, 357(2001).

- [7] T. Renger, and R. A. Marcus, J. Chem. Phys. **116**, 9997(2002).
- [8] A. Omerzu, M. Licer, T. Mertelj, V. V. Kabanov, and D. Mihailovic, Phys. Rev. Lett. **93**, 218101(2004).
- [9] R. Silbey, and R. A. Harris, J. Chem. Phys. **80**, 2615 (1984).
- [10] Z. Lü, and H. Zheng, Phys. Rev. B. **75**, 054302(2007); Q. Wang, A. Y. Hu, and H. Zheng, Phys. Rev. B. **80**, 214301(2009).
- [11] A. W. Chin, J. Prior, S. F. Huelga and M. B. Plenio, Phys. Rev. Lett. **107**, 160601 (2011).
- [12] S. Bera, S. Florens, H. U. Baranger, N. Roch, A. Nazir, A. W. Chin, Phys. Rev. B **89**, 121108(R) (2014); S. Bera, A. Nazir, A. W. Chin, H. U. Baranger, S. Florens, Phys. Rev. B **90**, 075110 (2014).
- [13] H. Zheng and Z. G. Lu, J. Chem. Phys. **138**, 174117 (2013); H. Zheng, Z. G. Lu, and Y. Zhao, arXiv:1407.2075 (2014).
- [14] Q. B. Ren and Q. H. Chen, Chin. Phys. Lett. **22**, 2914 (2005). Note that Eq. (7) here is just the superposition of two coherent states.
- [15] R. Bulla, N. H. Tong, and M. Vojta, Phys. Rev. Lett. **91**, 170601(2003); M. Vojta, N. H. Tong, and R. Bulla, Phys. Rev. Lett. **94**, 070604 (2005); R. Bulla, H. J. Lee, N. H. Tong, and M. Vojta, Phys. Rev. B. **71**, 045122(2005).
- [16] M. Vojta, N. H. Tong, and R. Bulla, Phys. Rev. Lett. **102**, 249904(E) (2009); M. Vojta, R. Bulla, F. Guttge, and F. Anders, Phys. Rev. B **81**, 075122 (2010).
- [17] F. R. Liu and N. H. Tong, Eur. Phys. J. B **86**, 141(2013).
- [18] For a review see: M. Vojta, Philos. Mag. **86**, 1807(2006).
- [19] A. Winter, H. Rieger, M. Vojta, and R. Bulla, Phys. Rev. Lett. **102**, 030601 (2009).
- [20] A. Alvermann and H. Fehske, Phys. Rev. Lett. **102**, 150601 (2009).
- [21] Y. Y. Zhang, Q. H. Chen and K. L. Wang, Phys. Rev. B **81**, 121105(R) (2010).
- [22] H. Wong, and Z. D. Chen, Phys. Rev. B. **77**, 174305(2008).
- [23] C. Guo, A. Weichselbaum, J. V. Delft, and M. Vojta, Phys. Rev. Lett. **108**, 160401 (2012).
- [24] M. F. Frenzel and M. B. Plenio, New Journal of Physics **15**, 073046(2013).
- [25] A. Osterloh et al., Nature (London) **416**, 608 (2002).
- [26] L. W. Duan, H. Wang, Q. H. Chen, and Y. Zhao, J. Chem. Phys. **139**, 044115 (2013); N. Wu, L. Duan, X. Li, and Y. Zhao, J. Chem. Phys. **139**, 084111 (2013).